FYS3150 project 4 - Ising model

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November 19, 2017

Abstract

A numerical study on the temperature dependency of ferromagnets in accordance with the Ising model has been conducted by utilizing the Monte Carlo method and the Metropolis algorithm [1]

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[1] full repository at https://github.com/mikaelbk/fys3150-project4

1 Introduction

In its essence, the two dimensional Ising model of a ferromagnet takes into consideration a lattice of dipoles that can either be spin up or spin down. A ferromagnet can reduce its internal energy by aligning spins (consequentially yielding a net magnetization), however, at higher temperatures, the 'randomizing' effects of entropy dominates. A description of the interplay between these to effects is achieved through Helmholtz free energy; and a thermodynamic equilibrium is reached when this free energy is minimized. The experimental results illustrates how the energy at equilibrium[2] changes as a function of temperature and also the relative relaxation time for different systems. The simple 2x2 lattice is first considered as, in contrast to the general case[3], it is relatively simple to solve it analytically. This allows for a comparison between analytical and numerical results. Later we solve for lattices of increasing size, which greatly increases complexity and computational requirements.

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[2]More specifically the average energy values sampled for a system over a significant period of time

[3]A general analytical solution of the partition function for the two-dimensional Ising model on a square lattice was solved in the 1940s by Lars Onsager. This approach however is way beyond the scope of this project. [1, p. 343]

2 Theory

2.1 The Ising Model

In the two dimensional Ising model we consider a lattice of dipoles that are allowed one of two spins, up or down. This restriction means that the model does break down to some degree at low temperatures, but fortunately is more accurate near the Curie temperature.[1, p. 340] It does not take into account long range interactions but rather each dipole interacts with its neighbors, four in our 2D case. Despite its simplicity the model does manage to predict the phase transition where the ferromagnet becomes a paramagnet at a sufficiently high critical temperature, famously called the Curie temperature, T_C.

2.2 Analytical solution of energies for the 2x2 lattice

In the following will be considered a 2x2 lattice with spins labeled A,B,C and D that is either spin up or spin down.

A	B
C	D

Let spin up and spin down be represented by the numbers 1 and -1 respectively. This makes sense when summing over nearest neighbour spin interactions when calculating the energy since opposite spins sum out to zero and equal spins contribute an equal amount of energy (say J) no matter the order. Due to symmetries, most energies cancel out and sum out to zero. Let's look at the ones that don't do this:

$$E = -J \sum_{kl}^{N} s_k s_l \neq 0$$

$$-J(A(B+C) + B(A+D) + C(A+D) + D(B+C)) \neq 0$$

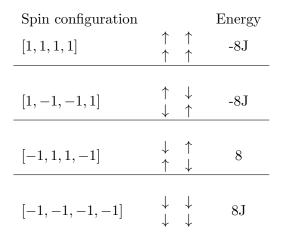$$A(B+C) + D(B+C) + B(A+D) + C(A+D) \neq 0$$

$$(A+D)(B+C) + (B+C)(A+D) \neq 0$$

$$2(A+D)(B+C) \neq 0$$

$$A + D \neq 0 \qquad B + C \neq 0$$

$$\implies A = D \quad \text{and} \quad B = C$$

Here it is assumed that $J \neq 0$ in the division. We use the fact that no factor can be zero when the product is nonzero and, for the last step, we use that the variables can only assume the values 1 or -1. So the only microstates with non-zero energies are

Spin configuration		Energy
$[1, 1, 1, 1]$	↑ ↑ ↑ ↑	-8J
$[1, -1, -1, 1]$	↑ ↓ ↓ ↑	-8J
$[-1, 1, 1, -1]$	↓ ↑ ↑ ↓	8
$[-1, -1, -1, -1]$	↓ ↓ ↓ ↓	8J

Where the energies are calculated by using formula INSERT using periodic boundary conditions. Because the total number of microstates is 2^{2n} in an nxn lattice there must be 12 other microstates with zero energy.

2.3 Analytical expressions for expectation values in 2x2 lattice

Finding expectation values is made a lot easier if you have the partition function. Fortunately it is trivial to find it in this specific case as we already have all the energies for the relatively few number of microstates. The partition function is defined as

$$Z = \sum i e^{-\beta E_i} \tag{1}$$

Which is a sum over all microstates with their corresponding energies and β is a variable that is inversely related to temperature. In our case the partition function is

$$Z = 2e^{8J\beta} + 2e^{-8J\beta} + 12$$

Now that we have the partition function we can calculate common expectation values, starting with the energy

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta}$$
$$= -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$$
$$= -\frac{8\big(Je^{8J\beta} - Je^{-8J\beta}\big)}{e^{8J\beta} + e^{-8J\beta} + 6}$$

There is a certain symmetry in the system as it has no way of differentiating between spin up or spin down. From this it follows that the

expectation value for magnetization, $\langle M \rangle$, must be zero. As is common in such cases we calculate the square and absolute value instead. The magnetization for a microstate M_i is calculated simply by taking a sum over all the spins in this state.

$$|M_i| = A_i + B_i + C_i + D_i$$

Since two spin up and two spin down yields a net zero magnetization these states do not contribute to the expectation value directly. We are left with the states where all spins are aligned and states where there is a single spin pointing in the opposite direction to the others. Observing that there are four states where a single spin is down and the same for spin up we realize that the multiplicity for states with a single spin misaligned must be 8. We already know all energies for the various states and conveniantly enough it appears that for states with equal absolute/squared magnetization they also have equal energies.

microstate	multiplicity	$|M|$	M^2	E_i
all aligned	2	4	16	-8J
single spin misaligned	8	2	4	0

$$\langle |M| \rangle = \tfrac{1}{Z} \sum_i |M_i| e^{-\beta E_i} = \frac{2(4e^{8J\beta}) + 8(2e^0)}{Z} = \frac{4e^{8J\beta} + 16}{e^{8J\beta} + e^{-8J\beta} + 6}$$

$$\langle M^2 \rangle = \tfrac{1}{Z} \sum_i M_i^2 e^{-\beta E_i} = \frac{2(16e^{8J\beta}) + 8(4e^0)}{Z} = \frac{16\left(e^{8J\beta} + 1\right)}{e^{8J\beta} + e^{-8J\beta} + 6}$$

The magnetic susceptibility comes out quite nicely from the following relation

$$\chi = \beta\left(\langle M^2 \rangle - \langle M \rangle^2\right) = \beta \frac{16\left(e^{8J\beta} + 1\right)}{e^{8J\beta} + e^{-8J\beta} + 6}$$

For the specific heat capacity we get

$$\langle C_v \rangle = -\frac{1}{kT^2} \frac{\partial}{\partial} \tag{2}$$

3 Results

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4   Conclusion

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References

[1] Daniel V. Schroeder, *An introduction to thermal physics*, San Francisco, Calif.: Addison Wesley Longman, 2005